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Low-energy excitations of the one-dimensional half-filled $SU(4)$ Hubbard model with an attractive on-site interaction: Density-matrix renormalization-group calculations and perturbation theory

Jize Zhao and Kazuo Ueda
Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan

Xiaoqun Wang
Department of Physics, Renmin University of China, Beijing 100872, China

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We investigate low-energy excitations of the one-dimensional half-filled $SU(4)$ Hubbard model with an attractive on-site interaction $U < 0$ using the density matrix renormalization group method as well as a perturbation theory. We find that the ground state is a charge density wave state with a long range order. The ground state is completely incompressible since all the excitations are gapful. The charge gap which is the same as the four-particle excitation gap is a non-monotonic function of U, while the spin gap and others increase with increasing $|U|$ and have linear asymptotic behaviors.

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The Hubbard model is one of the most classic models for strongly correlated electronic systems and has attracted long-term interest since the pioneering work in 1960s[1]. By taking the on-site Coulomb interaction into account, it well explains the puzzle that some materials with half-filled band are insulators. However, this model which consider only a single band, on-site Coulomb interaction and the nearest-neighbor hopping is often thought being oversimplified. To account for other features beyond the Mott physics[2], there are two kinds of natural extensions: one is to incorporate the orbital degree of freedom which may be called multi-band Hubbard model[3], and the other is to consider the hopping and/or the Coulomb interaction with longer ranges.

In the last several years, ultra-cold atomic experiments evoke systematic studies of correlation effects in the optical lattice systems where interactions are tunable through Feshbach resonance. The Hubbard model becomes again an appropriate one to envisage some relevant issues with both positive and negative interactions. Recently, fermionic atoms with higher spins are successfully trapped into optical lattices [4]. This calls for a generalization of the $SU(2)$ Hubbard model into the $SU(N)$ case[5, 6]. In this paper, we study one-dimensional $SU(4)$ Hubbard model which is represented as

$$\mathcal{H} = -t\sum_{i=1}^{L}\sum_{\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma}+h.c.)+\frac{U}{2}\sum_{i=1}^{L}\sum_{\sigma\neq\sigma'}n_{i\sigma}n_{i\sigma'} \quad (1)$$

where $t > 0$ is a hopping matrix element, L the number of the lattice sites, σ and $\sigma^{'}$ the spin indices taking $-\frac{3}{2}$, $-\frac{1}{2}$, $\frac{1}{2}$ and $\frac{3}{2}$. $c_{i\sigma}^{\dagger}(c_{i\sigma})$ denotes the creation(annihilation) operator of a particle with spin σ at the site i, $n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma}$ is the corresponding number operator and U is the on-site interaction.

This model is not exactly solvable even in one dimension in contrast to the $SU(2)$ case[7, 8]. Nevertheless, some aspects of physical properties can be reliably explored by some analytical approaches as well as numerical methods such as density matrix renormalization group (DMRG)[9, 10] and Quantum Monte Carlo simulations[11, 12]. Most recently, an $SO(8)$ symmetry regime was proposed between $0 < U < 3t$ at half-filling by Assaraf et al[12] with using a nonperturbative renormalization group method and quantum Monte Carlo simulation. They found that the low-energy spectrums are gapful in this regime. The similar results were also shown later by Szirmai and Sólyom for the other $N > 2$ case[13]. Those studies were concentrated on the repulsive case $U > 0$, but for the $U < 0$ case few results are obtained so far. On the other hand, it is well known that the one-dimensional attractive half-filled $SU(2)$ Hubbard model is described by a Luther-Emery liquid[14], in which the charge excitation is gapless, whereas the spin excitation is gapful. By the hidden $SU(2)$ transformation the $SU(2)$ Hubbard model with U can be mapped to the one with $-U$, while for the $SU(4)$ case such a mapping does not exist so that one cannot obtain any insights into the low-energy properties through the mapping. In this paper, we will show that the $SU(4)$ Hubbard model at half-filling with the attractive interaction belongs to a different universality class from the $SU(2)$ one.

Let us start with a perturbation theory for the strong coupling regime. For this purpose, we rewrite the Hamiltonian (1) as $\mathcal{H} = \mathcal{H}_t + \mathcal{H}_u$, where the hopping term $\mathcal{H}_t = -t\sum_{i\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma} + h.c.)$ is regarded as a perturbation and the on-site interaction $\mathcal{H}_u = \frac{U}{2}\sum_{i\sigma\neq\sigma'}n_{i\sigma}n_{i\sigma'}$ as the zeroth order Hamiltonian has highly degenerate ground states in which each site is either fully occupied by four particles forming a $SU(4)$ singlet, or empty. Up to the second-order, the effective Hamiltonian is given by

$$\mathcal{H}_{eff}^{(2)} = \frac{2t^2}{3U}P\sum_{i}n_iP - \frac{t^2}{6U}P\sum_{i}n_in_{i+1}P, \quad (2)$$

where P is a projection operator which projects a state onto the subspace spanned by the ground states of $\mathcal{H}_u$, and $n_i = \sum_\sigma n_{i\sigma}$ the number operator at the site i. The hopping term $\mathcal{H}_t$ lifts the degeneracy of $\mathcal{H}_u$ and gives rise to both the energy gain of $\frac{4t^2}{3U}$ per site at half-filling as denoted by the first term of (2) and an effective repulsive interaction between particles on the nearest-neighbor sites as denoted by the second term of (2). The second term induces essentially a charge-density-wave (CDW) ground state with a true long range order such that every other site is fully occupied with an empty site in between, which is consistent with the mean field result for the weak coupling region[6]. Moreover, $\mathcal{H}^{(2)}_{eff}$ has two-fold degenerate ground states, each of which is a $SU(4)$ singlet.

An important question concerning the CDW ground state is whether it is metallic or insulating. To address this question, we need to examine charge excitations. The charge gap Δ_c is the energy difference of the lowest excitation in the spin singlet channel from the ground state as defined by $\Delta_c = E_1(L, 2L, 0) - E_0(L, 2L, 0)$, in which $E_n(L, N, S)$ stands for the the $n-$th excitation energy in a spin-S channel with L sites and N particles. And another interesting issue is to explore the relevance of the four-particle excitation gap Δ_4 to Δ_c for the $SU(4)$ symmetry. Δ_4 represents the energy cost of adding four particles or holes into the systems such that $\Delta_4 = \frac{1}{2}[E_0(L, 2L+4, 0) + E_0(L, 2L-4, 0) - 2E_0(L, 2L, 0)]$. From $\mathcal{H}^{(2)}_{eff}$, one can easily find $\Delta_c = -\frac{8t^2}{3U}$ based on the fact that the motion of four particles from one of fully occupied sites to its neighbor costs a minimal energy. Similarly, adding four particles to the system would gain the energy $6U+2\times(-\frac{8t^2}{3U})$, while adding four holes costs $-6U$, thus one has $\Delta_4 = -\frac{8t^2}{3U}$. It turns out that the four-particle excitation gap is essentially the same as the charge gap and finite.

However, the situation is completely different for the $SU(2)$ case, where the ground state is metallic. To understand this, one can write the effective Hamiltonian in the strong coupling limit for the $SU(2)$ case as[15]:

$$\begin{aligned} \mathcal{H}^{(2)}_{eff,su(2)} &= \frac{2t^2}{U} P \sum_{i\sigma} n_{i\sigma} P \\ &- \frac{t^2}{U} P \sum_{\langle ij\rangle\sigma} (n_{i\sigma} n_{j\sigma} - c^+_{i\sigma} c^+_{i\bar{\sigma}} c_{j\bar{\sigma}} c_{j\sigma}) P. \end{aligned} \tag{3}$$

This Hamiltonian distinguishes itself from $\mathcal{H}^{(2)}_{eff}$ with its last additional term which allows a "pair hopping" process between the two neighbor sites. Although the second repulsive term would be in favor of forming a CDW ground state with gapful charge excitations, the extra "pair hopping" term eventually destabilizes this CDW long range order resulting in gapless charge excitations. On the other hand for the $SU(4)$ case, similar hopping term can only appear after calculating to higher order. Therefore, the perturbation theory in the strong coupling regime shed light on the different nature of the ground states between the $SU(2)$ and $SU(4)$ cases.

In order to go beyond the validity range of the above perturbation theory for a full exploration of the low-energy properties, we have performed systematic DMRG computations. There are actually some difficulties inherent to this model, such as a large number of degrees of freedom for each site and different edge states so that some measures are taken necessarily to reach sufficient accuracy in our computations. To calculate Δ_c, we have to use the periodic boundary condition (PBC) with the even number of sites because of multi-edge excitations in the $SU(4)$ singlet subspace when open boundary condition (OBC) is imposed. For other gaps, we can efficiently expel the corresponding edge excitations by an OBC algorithm. In particular, one lattice site is added at each step and broken into two pseudo-sites. When the infinite system algorithm is conducted with the size of the superblock up to some odd number of sites L which are preselected, the sweeping procedure is performed for those L. The necessary extrapolations for the thermodynamic limit are finally made properly on the data with these preselected sites. In this case, we have to redefine the gaps correspondingly, for instance $\Delta_4 = E_0(L, 2L+6, 0) - E_0(L, 2L+2, 0) - 6U$, where the particle-hole symmetry is explicitly taken into account. In the strong coupling region, PBC is often used to identify the bulk values of a gap rather than edge-excitation energy obtained under OBC. In our computations, t is set to be unit and 2000 states are kept for most cases and the maximal truncation error is the order of 10^{-7}.

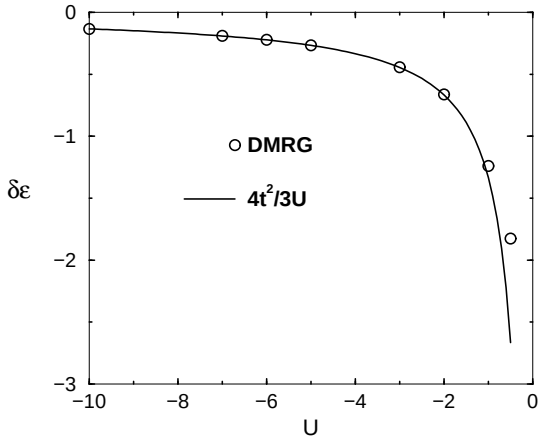

FIG. 1: Ground state energy correction per site from $\mathcal{H}^{(2)}_{eff}$ (solid line) versus U in comparison with DMRG data (◯).

Figure 1 displays the ground state energy correction per site arising from the hoping term for the thermodynamic limit. Both the numerical results and the perturbation theory show this energy increases monotonically

as $|U|$ increases and approaches to zero asymptotically. When $-2 < U < 0$, the results of the perturbation theory deviates from DMRG ones, and the deviation becomes significant for small $|U|$. This is reasonable because in this region the hopping term $\mathcal{H}_t$ is no longer perturbative. However, for $U < -2$, the perturbation theory provides very good results which accurately agrees with the DMRG data. On the other hand, our DMRG calculations with both OBC and PBC show that for a finite and even L, the ground state is unique and a $SU(4)$ singlet which belongs to the irreducible representation $[1^4][16]$. In addition, slightly above the ground state there is one accompanied $SU(4)$ singlet excited state, whose energy difference from the ground state diminishes as $L \to \infty$. Therefore, one obtains two-fold degenerate ground states in the thermodynamic limit, which are consistent with our analysis based on $\mathcal{H}^{(2)}_{eff}$. These degenerate CDW ground states with the long range order result from the translational symmetry breaking.

In FIG. 2, we show the DMRG results on the charge gap Δ_c and the four-particle excitation gap Δ_4 for the entire range of $U < 0$. First of all, one can see that both Δ_c and Δ_4 are non-vanishing for all finite $U < 0$ so that the ground state is insulating rather than metallic in contrast to the $SU(2)$ case. Secondly, these two gaps behave non-monotonically with U. The maximum shown around $U = -2$ indicates a crossover region between weak and strong interaction regimes. Third, the perturbation theory for the strong coupling regime provides correctly the asymptotic behavior for large $|U|$ limit and shows a qualitative agreement with the DMRG results in the strong coupling regime. The visible deviation from the DMRG results sets on at about $U \approx -5$ lower than that ($U \approx -2$) for the ground state energy correction shown in Fig. 1. In the weak coupling regime, Δ_c and Δ_4 shown by DMRG decrease with increasing U. Finally, while $\mathcal{H}^{(2)}_{eff}$ can predict $\Delta_c = \Delta_4$ only in the strong coupling limit, our DMRG calculations show that within the numerical accuracy Δ_c remains equal to Δ_4 beyond the strong coupling regime. Although it is difficult from the DMRG calculations to obtain sufficiently accurate Δ_c for $-1 < U < 0$ yet, it is reasonable to conclude that Δ_4 is equal to Δ_c for all $U < 0$ in the $SU(4)$ case.

Now we turn to the other three types excitations: the first one is the quasi-particle gap Δ_1 for adding single particle or single hole to the system, the second one spin gap Δ_s corresponding to the excitation energy in the spin triplet channel from the ground state, and the last one two-particle gap Δ_2 defined as energy cost when two particles or two holes are added to the system. While these three gaps together with Δ_c and Δ_4 essentially involve all kinds of relevant excitations, they have significantly different behaviors. Since the ground state is the CDW state with the long range order, it is insightful to analyze those excitations in the Hartree-Fock (HF) approximation. The CDW state in HF approximation can be achieved by simply writing the on-site interaction as $n_{i\sigma}n_{i\sigma'} \approx \langle n_{i\sigma}\rangle n_{i\sigma'} + n_{i\sigma}\langle n_{i\sigma'}\rangle - \langle n_{i\sigma}\rangle\langle n_{i\sigma'}\rangle$ and assuming $\langle n_{i\sigma}\rangle = n + (-1)^i\delta n$, where n is the average number of particles per site for each spin and δn the corresponding order parameter. At half-filling, one has $n = \frac{1}{2}$ and $0 \le \delta n \le \frac{1}{2}$. By further introducing $a_{l\sigma} = c_{2l\sigma}$ and $b_{l\sigma} = c_{2l+1\sigma}$ for each sublattice of the bipartite lattice, respectively, and taking the Fourier transformation, then we can write down the Hartree-Fock Hamiltonian as:

$$\begin{aligned}\mathcal{H}^{HF} &= -t\sum_{k\sigma}\left((1+e^{-ik})a^+_{k\sigma}b_{k\sigma} + h.c.\right) \\ &\quad +3U\delta n\sum_{k\sigma}(a^+_{k\sigma}a_{k\sigma} - b^+_{k\sigma}b_{k\sigma}) + const. \quad (4)\end{aligned}$$

Diagonalizing this Hamiltonian, one can obtain two bands for each spin species σ with the quasi-particle dispersions $w^{\pm}_{\sigma} = \pm\sqrt{\Delta_1^2 + 4t^2\cos^2\frac{k}{2}}$ where $\Delta_1 = -3U\delta n$. Moreover, one has $\Delta_c = \Delta_s = 2\Delta_1$ in the HF approximation. These gaps can be then evaluated after solving the following self-consistent equation $2\delta n = \langle a^+_{l\sigma}a_{l\sigma}\rangle - \langle b^+_{l\sigma}b_{l\sigma}\rangle$ for the order parameter δn. In order to calculate the two-particle excitation gap, however, it is necessary to account for the particle-particle correlations into the HF approximation, which is nothing but the random phase approximation (RPA). For this purpose, one first constructs the basis with two-particle excitations from the ground state of $\mathcal{H}^{HF}$ as follows:

$$|\Psi_{pp'\sigma}\rangle = \alpha^+_{p\sigma}\alpha^+_{p'\bar{\sigma}}|\Psi_g\rangle, \qquad |\Psi_g\rangle = \prod_{k\sigma}\beta^+_{k\sigma}|0\rangle) \quad (5)$$

where $\alpha^+_{p\sigma}$ is an operator creating one quasi-particle with momentum p and spin σ in the w^+ band and in $|\Psi_g\rangle$ the band w^-_{σ} is fully filled up by quasi-particles $\beta^+_{k\sigma}$ with the

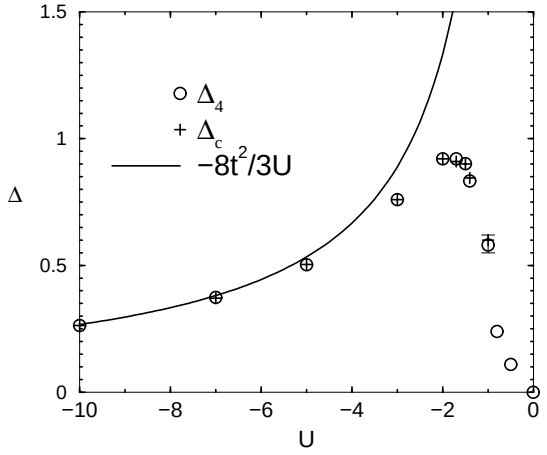

FIG. 2: DMRG results for charge gap (+) and four-particle gap (◯) versus U in comparison with perturbation ones (solid line). Error bars are smaller than size of symbols except for Δ_c at $U = -1$ as estimated with keeping different states.

momenta k and spin σ. Then Δ_2 can be obtained by diagonalizing $\mathcal{H}$ on the above basis (5).

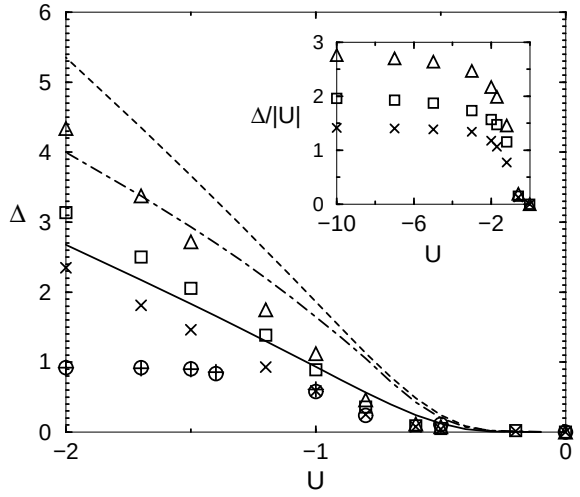

FIG. 3: DMRG results for one particle gap Δ_1 ($\times$), two-particle gap Δ_2($\Box$), spin gap Δ_s ($\triangle$), four-particle excitation gap Δ_4 ($\bigcirc$) and charge gap Δ_c(+) are shown as a function of U. The results of HF-RPA for Δ_1, Δ_2 and Δ_s denoted by solid, dot-dashed, and dashed lines, respectively. Inset shows $\Delta/|U|$ versus U for Δ_1 ($\times$), Δ_2 ($\Box$) and Δ_s ($\triangle$).

As compared to the DMRG results, we found that HF-RPA can provide a qualitatively correct description for Δ_1, Δ_2, and Δ_s. Figure 3 shows the DMRG data on all five gaps as well as Δ_1, Δ_2, and Δ_s from HF-RPA approximation for the region of $-2 \leq U \leq 0$ and the inset illustrates Δ_1, Δ_2, and Δ_s by showing ratios for them over $|U|$ up to $|U| = 10$. In contrast to Δ_c and Δ_4 as seen from Fig. 2, Δ_1, Δ_2, and Δ_s increase with increasing $|U|$ and become linear in large $|U|$ limit. It turns out that the relation $\Delta_c = \Delta_s$, given by the HF approximation, is invalid for general $U < 0$. Moreover, it is unclear but beyond the present approaches whether there is a symmetry enlargement similar to the one proposed for the repulsive case[12]. Nonetheless, HF-RPA presents precise asymptotic behaviors for Δ_1, Δ_2 and Δ_s. In the weak coupling limit, the exponential opening of these gaps can be well reproduced from the solution to the self-consistent equation $\delta n \sim -\frac{2\pi t}{3U} e^{\frac{2\pi t}{3U}}$ and with taking into account the two-particle correlations. In the strong coupling limit, one has $\Delta_1 \sim -1.5U$ and $\Delta_s \sim -3U$ from $\delta n \to 0.5$, and $\Delta_2 \sim -2U$ from the HF-RPA calculations[17]. The corresponding coefficients are in good agreement with the DMRG results as can be seen from the inset. On the other hand, the results of HF-RPA deviate from the DMRG data apparently in the intermediate coupling regime, but this is quite understandable since correlations involved in (1) cannot be accurately handled in HF-RPA when $\mathcal{H}_t$ and $\mathcal{H}_u$ become comparable, i.e. neither of them are perturbative.

In summary, we have studied the low energy properties of the one-dimensional half-filled $SU(4)$ Hubbard model with the attractive on-site interaction by using the DMRG method as well as the perturbation theory. We found that the ground state is a CDW insulating state with the long range order in which the translational symmetry is broken and all kinds of excitations are gapful for finite $U < 0$. Within our numerical accuracy, we found that the four-particle excitation gap is the same as the charge gap. While the charge gap (the four particle excitation gap) behaves non-monotonically, the others increase with increasing $|U|$ and have a linear-U asymptotic behavior with different coefficients. Therefore, we believe that the one-dimensional attractive half-filled Hubbard model for the $SU(4)$ and $SU(2)$ cases belong to different universality classes. Moreover, we find that the nature for the $SU(4)$ case can be further generalized to the other $SU(N > 2)$ cases[18]. At the end, it is worthwhile to mention that since the four-particle excitation gap as well as the charge gap are the smallest energy scale for the $SU(4)$ case with $U < 0$, it would be very interesting to detect four-particle process (excitations) in an ultracold fermionic atom system with the hyperfine spin-3/2.

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